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# New Center for Computational Sciences and Engineering Established

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**O**n Friday, November 12, the LLNL Computation Organization announced the formation of the Center for Computational Sciences and Engineering (CCSE). This new research center will be affiliated with the National Energy Research Supercomputer Center (NERSC) and report to me as NERSC's Director. The CCSE will function as a Lab-wide resource to promote the development of new mathematical algorithms and applications software for modeling complex physical phenomena on high-performance computer architectures.

Dr. John Bell will serve as director of the new Center. Bell was formerly head of the Applied Mathematics Group in the LLNL Computing and Mathematics Research Division (CMRD). Dr. Milo Dorr, former head of the Numerical Mathematics Group in CMRD, will serve as deputy director. The new Center will be initially staffed by 20 mathematicians, physicists and engineers from LLNL's applied mathematics research effort.

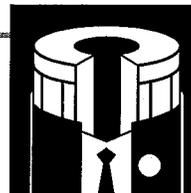
The core of the new Center will be LLNL's Applied Mathematical Sciences Program, which is funded by DOE's Office of Scientific Computing. Under this program, members of the CCSE already have collaborations with ER funded researchers, and with this new organization comes a commitment to starting more. In addition, the CCSE will become the home for existing collaborative projects that have traditionally provided applied mathematics support to LLNL Programs.

"The creation of the CCSE will also help the Lab respond to DOE's new emphasis on technology transfer and will enable us to reach out to industry to help solve

their important computational science problems," said Bell at the formal announcement of CCSE's creation. Two projects in the new Center reflect this new mission for LLNL. One of these projects is the LLNL component of a DOE High Performance Computing and Communication (HPCC) Grand Challenge Project on Computational Fluid Dynamics and Combustion Dynamics. In this project, researchers at LLNL along with collaborators at Los Alamos National Laboratory, University of California Berkeley, and the Courant Institute at New York University are developing sophisticated new modeling techniques for industrial combustion problems. For example, these new techniques could be used by an engineer to understand how pollutants are formed in an industrial burner.

Another industrially focused project, "Modeling Subsurface Flow and Chemical Migration on Massively Parallel Computers," is part of the DOE's Technology Transfer Initiative. In this project, LLNL researchers are working with the International Technology Corporation under a Cooperative Research and Development Agreement (CRADA) to develop new computational capabilities for modeling flow in heterogeneous porous media. The methodology being developed will enable detailed simulations of large sites which will play a key role in the design of remediation techniques to clean up contaminated groundwater at governmental and industrial sites throughout the world.

Bell indicated that these types of projects are typical of the opportunities available for Lab researchers to reach out to US industry. "One of our goals in forming the



Center for Computational Sciences and Engineering is to provide a focal point for multidisciplinary computational science projects that can aggressively pursue these types of new opportunities.”

I believe this partnership creates a powerful new research environment, and that joining the applications-driven algorithm development expertise in the CCSE with the high performance computing and networking expertise in NERSC will allow us to develop strong, new research opportunities. John Bell and Milo Dorr are, as always, ready to discuss opportunities for new projects with members of the ER research community.

At a meeting held to kick off the new Center, Bill Lokke, LLNL Associate Director for Computations, said, “The combination of these capabilities creates a new partnership of research and high-performance computing for the Laboratory. It positions the Computation Organization to be more responsive to DOE's multiple missions.”

